Chapter 2
Riding the Wave: More on Wave Mechanics

2.1 Units of Measure

Many quantum mechanics (QM) references ignore the units of measure of the components of a calculation. For example, the most common element of QM calculations is the one-dimensional (1D) x-representation wave-function, $\psi(x)$. What are its units? Answer: $\mathrm{m}^{-1/2}$, or per-square-root-meters. Surprised? So were we.

In the following, we use square brackets to mean “the units of.” For example, $[x]$ means “the units of x.”

Let us start with the basics: in the macroscopic universe there are exactly four fundamental quantities: distance, mass, time, and charge. (One can reasonably argue for a fifth: angle.) In the MKSA system, the corresponding units are meters (m), kilograms (kg), seconds (s), and coulombs (C). We stick mostly with MKSA in this text. As is common, we use the terms “units” and “dimensions” interchangeably in this context.

For the units of $\psi(x)$, recall that the dot product of a normalized wave-function with itself is a dimensionless 1:

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)\, dx = 1 \qquad (\text{dimensionless})$$

Since dx is in meters (m) and the units of ψ^* are the same as ψ, then $\psi^*\psi$ must be in m^{-1}, and thus ψ is in $\mathrm{m}^{-1/2}$.

Equivalently, if x is in meters and we compute the average of x:

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, x\, \psi(x)\, dx,$$

then the units of ψ must be $\mathrm{m}^{-1/2}$.

What about the momentum representation, $a(p)$? The same normalization process starts with

$$\int_{-\infty}^{\infty} a^*(p)a(p)\, dp = 1 \quad (\text{dimensionless}) \quad \text{where} \quad p \text{ is in } \frac{kg \cdot m}{s}.$$

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Then $a(p)$ must be in $\left[\text{momentum}\right]^{-1/2} = \left[\dfrac{s}{kg \cdot m}\right]^{1/2}$, or $s^{1/2}\ kg^{-1/2}\ m^{-1/2}$, or "inverse square-root momentum."

Recall that mathematically, exponentials and logarithms are dimensionless and their arguments must be dimensionless. Also, the unit "radian" is equivalent to dimensionless, because it is defined as arc-length/radius = m/m = dimensionless.

What about three-dimensional (3D) wave-functions? Given $\psi(x, y, z)$, its units are $m^{-3/2}$. Why? We refer again to the normalization integral, which says that the particle must be somewhere in the universe, i.e.,

$$\Pr(\text{particle is somewhere in the universe}) = 1$$
$$= \iiint_{universe} \psi^* \psi \, dx\, dy\, dz \quad (\text{dimensionless}).$$

The units of $dx\,dy\,dz$ are m^3, so ψ must be in $m^{-3/2}$. Often, for spherically symmetric potentials, ψ is a function of r, ϕ, and θ: $\psi(r, \theta, \phi)$. Then it must have units of $m^{-3/2}\ rad^{-1}$:

$$\iiint_{universe} \psi^* \psi r^2 \sin\theta \, dr\, d\phi\, d\theta = 1 \quad \text{and} \quad r^2\, dr\, d\phi\, d\theta \text{ is in } m^3\text{-rad}^2.$$

However, since rad is dimensionless, this is the same as before: $m^{-3/2}$. Thus, as expected, the units of ψ are independent of the units of its arguments.

The unit of two-dimensional (2D) $\psi(x, y)$ is left as an exercise for the reader.

2.1.1 *Dimensions of Operators*

> Operators also have dimensions.

Let us consider the momentum operator. $\dfrac{d}{dx}$ is like dividing by x, so it has units of (1/m), or m^{-1}. Planck's constant h, or $\hbar \equiv h/2\pi$, is a quantum of action, (energy) (time), or of angular momentum (distance) (momentum); the units are thus joule-seconds (J-s), or in purely fundamental terms, kg-m²/s. Then:

$$\hat{p} = \frac{\hbar}{i}\frac{d}{dx} \quad \Rightarrow \quad \text{units of} \left(\frac{kg \cdot m^2}{s}\right)\left(\frac{1}{m}\right) = \frac{kg \cdot m}{s}, \qquad \text{consistent with } p = mv.$$

The momentum operator has units of momentum.

In fact, all observable operators have the units of the observable. We can see this from the average value formula:

$$\langle \hat{o} \rangle = \int_{\infty} \psi^* \hat{o} \psi \, dx, \qquad \text{and} \qquad [\psi^* \psi \, dx] = \text{dimensionless} \quad \Rightarrow \quad [\hat{o}] = [o].$$

When composing operators, their units multiply. Thus, we see that $\dfrac{d^2}{dx^2}$ has units of m^{-2}, etc.

Commutators are compositions of other operators, so the units of commutators are the composition of the units of the constituent operators. (More on commutators elsewhere.) Perhaps the most famous quantum commutator is:

$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar.$$

The units of $\hat{x}$ are m. (Note that the units of $\hat{x}\psi(x)$ = $\mathrm{m}(\mathrm{m}^{-1/2}) = \mathrm{m}^{1/2}$, *not* m.) The units of $\hat{p}$ are kg-m/s. The units of $\hat{x}\,\hat{p}$ are simply the product of the units of $\hat{x}$ and $\hat{p}$: $(\mathrm{m})(\mathrm{kg\text{-}m/s}) = \dfrac{kg \cdot m^2}{s}$. This must be, because the commutator in this case works out to a constant, $i\hbar$, with those units.

Note that the units of operators do not change with the representation basis. For example, $\hat{x}$ in the momentum representation is still meters:

$$\hat{x} = i\hbar \frac{d}{dp} \qquad \Rightarrow \qquad \text{units of} \left[\frac{\dfrac{\mathrm{kg\ m^2}}{\mathrm{s}}}{\dfrac{\mathrm{kg\ m}}{\mathrm{s}}} \right] = \mathrm{m}.$$

2.2 The Dirac Delta Function

The Dirac delta function is used heavily all over physics, engineering, and mathematics. Thoroughly understanding it is essential for anyone in those fields. Read more about the δ-function in *Funky Mathematical Physics Concepts* (http://physics.ucsd.edu/~emichels/FunkyMathPhysics.pdf). The δ-function is also called an "impulse" or "impulse function."

The Dirac delta function is really a pseudofunction: it implies taking a limit, but without the bother of writing "$\lim_{\Delta x \to 0}$" all the time. The Dirac delta function is often formally defined as the limit of a Gaussian curve of (a) infinitesimal width, (b) unit integral $\left(\int_{-\infty}^{\infty} \delta(x)\, dx = 1 \right)$, and thus (c) infinite height. This is somewhat overkill for our purposes, and it may be simpler to think of the delta function as a *rectangular* pulse of (a) infinitesimal width, (b) unit area, and thus (c) infinite height, located at zero (Fig. 2.1, *left*):

Mathematically, we could write this *simplified* (asymmetric) delta function as

$$\text{simplified } \delta(x) = \lim_{\Delta x \to 0} f(x) \qquad \textit{where} \qquad \begin{aligned} f(x) &= 0, && x < 0 \\ f(x) &= 1/\Delta x, && 0 \le x \le \Delta x \\ f(x) &= 0, && x > \Delta x. \end{aligned}$$

Though the previous works for any well-behaved (i.e., continuous) function, the delta function is usually considered an even function (symmetric about 0), so it is sometimes better to write (Fig. 2.1, *right*):

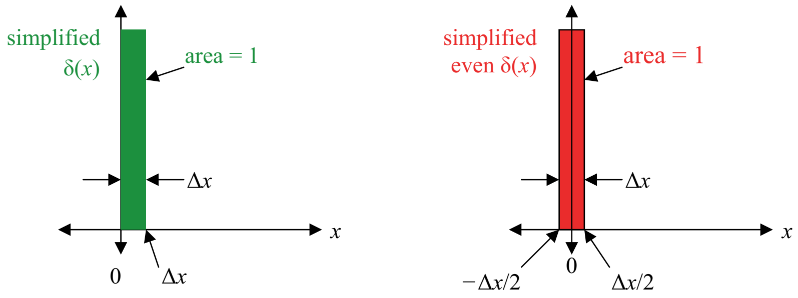

Fig. 2.1 (*Left*) The δ-function can be written as one-sided in most cases. However, (*right*) it is usually considered even. In any case, we take the limit as $\Delta x \to 0$

$$\text{simplified } \delta(x) = \lim_{\Delta x \to 0} f(x) \qquad \textit{where} \qquad \begin{array}{ll} f(x) = 0, & x < -\Delta x/2 \\ f(x) = 1/\Delta x, & -\Delta x/2 \le x \le \Delta x/2 \\ f(x) = 0, & x > \Delta x/2. \end{array}$$

However, in spherical polar coordinates, the radial delta function at zero requires the *asymmetric* form, and cannot use the symmetric form (see *Funky Mathematical Physics Concepts*).

Both of the previous simplified versions of the delta function require special handling for more advanced applications where we need to take derivatives of $\delta(x)$; we will not use such derivatives in this book.

2.2.1 Units of the Delta Function

Another surprise: the δ-function is *not* dimensionless.

The Dirac delta function has units!

Usually, such mathematically abstract functions are dimensionless, but the key property of the delta function is that its *area* is 1 and dimensionless. This means:

$$\int_{-\infty}^{\infty} \delta(x)\, dx = 1 \quad \text{(dimensionless)}.$$

So if x (and thus dx) is in m, $\delta(x)$ must be in m^{-1}. But we use the delta function for all sorts of measures, not just meters: radians, momentum, etc. So by definition, the delta function assumes units of the inverse of its argument. Given a radian, the units of $\delta(\theta)$ are inverse radians (rad^{-1}, equivalent to dimensionless); given a momentum, the units of $\delta(p)$ are $\frac{s}{kg \cdot m}$; and so on. Also, $\delta^{(3)}(\mathbf{r})$ has units of the inverse cube of the units of $\mathbf{r}$ ($\mathbf{r}$ in m $\Rightarrow \delta^{(3)}(\mathbf{r})$ in m^{-3}), and $\delta^{(4)}(x^\mu)$ has units of the inverse fourth power of the units of x^μ.

An important consequence of the definition of $\delta(x)$ is that, because $\delta(x)=0$ except near $x=0$,

$$\int_{-\varepsilon}^{\varepsilon} \delta(x)\, dx = 1, \qquad \forall \varepsilon > 0.$$

Note that $\delta(x)$ is *not* square integrable, because

$$\int_{-\infty}^{\infty} \delta^2(x)\, dx = \lim_{\Delta x \to 0} \int_0^{\Delta x} \left(\frac{1}{\Delta x}\right)^2 dx = \lim_{\Delta x \to 0} \left[\frac{x}{(\Delta x)^2}\right]_0^{\Delta x} = \lim_{\Delta x \to 0} \frac{1}{\Delta x} \to \infty.$$

Interestingly, though the delta function is often given as a Gaussian curve, the precise form does not matter, so long as it is analytic (i.e., infinitely differentiable or has a Taylor series), unit integral, and infinitely narrow [15, p. 479b]. Other valid forms are:

$$\delta(x) = \lim_{\lambda \to 0} \frac{1}{\pi} \frac{\lambda}{\lambda^2 + x^2}, \qquad\qquad \delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx}\, dk.$$

This latter form is extremely important in quantum field theory, and QM in the momentum representation.

2.2.2 *Integrals of δ-Functions of Functions*

When changing variables, we sometimes need to know what is $\int dx\ \delta\big(f(x)\big)$?

$$\text{Let} \qquad u = f(x), \quad du = f'(x)\, dx \quad \text{and define } x_0 \ s.t. \quad f(x_0) = 0.$$

$$\text{Then} \quad \int_{-\varepsilon}^{\varepsilon} dx\ \delta(f(x)) = \int_{-\varepsilon'}^{\varepsilon'} du \frac{1}{|f'(x_0)|} \delta(u) = \frac{1}{|f'(x)|}.$$

We must take the magnitude of the derivative, because $\delta(x)$ is always positive, and always has a positive integral. The magnitude of the derivative scales the area under the delta function.

If the interval of integration covers multiple zeros of $f(x)$, then each zero contributes to the integral:

$$\text{Let} \qquad x_i = \text{zeros of } f, \text{ i.e. } f(x_i) = 0, \quad i = 1, \ldots n.$$

$$\text{Then} \quad \int_{-\varepsilon}^{\varepsilon} dx\ \delta(f(x)) = \sum_{i=1}^{n} \frac{1}{|f'(x_i)|}.$$

2.2.3 3D δ-function in Various Coordinates

See *Funky Mathematical Physics Concepts* for a more complete description, but note that $\delta^3(\mathbf{r})$ has a simple form *only* in rectangular coordinates:

$$\delta^3(x, y, z) = \delta(x)\delta(y)\delta(z),$$

but:

$\delta^3(r, \theta, \phi) \neq \delta(r)\delta(\theta)\delta(\phi)$. (It is more complicated than this.)

2.3 Dirac Notation

Dirac notation is a way to write the **algebra** of QM bras, kets, and operators. It is widely used, and essential to all current QM. It applies to both wave-mechanics and discrete-state mechanics (discussed in a later chapter).

You are familiar with the ordinary algebra of arithmetic. You may be familiar with Boolean algebra. There are also algebras of modular arithmetic, finite fields, matrix algebra, vector spaces, and many others. All algebras are similar to arithmetic algebra in some ways, but each is also unique in some ways. In general, an **algebra** is a set of rules for manipulating symbols, to facilitate some kind of calculations. We here describe Dirac notation and its associated Dirac algebra. Included in Dirac algebra is the algebra of operators (covered in a later section). Dirac algebra also brings us closer to the concept of kets and bras as vectors in a vector space (see p. 81).

2.3.1 Kets and Bras

For wave mechanics, **kets** and **bras** are complex-valued functions of space (spatial functions), such as quantum states, and the results of operators on states. In Dirac notation, kets are written as $|name\rangle$, where "name" identifies the ket. The ket is a shorthand for the spatial wave-function, say $\psi(\mathbf{r})$. The "name" is arbitrary, much like the choice of letters for variables in equations. However, there are some common conventions for choosing ket names, again similar to the conventions for using letters in equations. In this section, we discuss only the spatial kets.

As a ket example, suppose we have a 1D spatial wave-function, $\psi(x)$. Since any wave-function can be written as a ket, we might write the ket for $\psi(x)$ as $|\psi\rangle$ (assuming some notational license for now):

$$|\psi\rangle \equiv \psi(x) = \text{complex-valued function of } x.$$

Note that the ket $|\psi\rangle$ stands for the *whole* wave-function; it does *not* represent the value of the wave-function at any particular point. One of the key benefits of Dirac notation is that *kets, bras, and operators are independent of any representation basis*.

Since they always represent the *entire* spatial function, there's no question of "what is the basis for a ket?" More on representations (decomposition in different bases) later.

Some might object to equating a ket to a function, as we did previously: $|\psi\rangle = \psi(x)$. More specifically, $\psi(x)$ is a particular representation of the quantum state $|\psi\rangle$, so it would perhaps be more explicit to say "$|\psi\rangle$ can be represented as $\psi(x)$," but that seems pedantic. We all agree that "5 = 4 + 1," yet the symbol "5" is different than the symbol "4 + 1." They are two representations of the same mathematical quantity, 5. Furthermore, since any function of position, say $\psi_x(x)$, can be written as a function of momentum, $\psi_x(x)$, our flexible notation would say that $\psi_x(x) = \psi_p(p)$, which is OK with us. This simply means that $\psi_x(x)$ and $\psi_p(p)$ both represent the same mathematical entity. I am therefore content to say:

$$|\psi\rangle = \psi_x(x) = \psi_p(p) = \text{any other representation of the ket } |\psi\rangle.$$

Dual to kets are **bras**. Bras are written as $\langle name|$, where "*name*" identifies the bra. Bras are also a shorthand for complex-valued functions of space. The same function of space can be expressed as either a ket or a bra. The difference is the ket is shorthand for the spatial function itself; the bra is shorthand for the complex conjugate of the function. Thus (continuing our flexible notation),

$$\langle\psi| = \psi^*(x) \qquad (\text{complex conjugate}).$$

For example, suppose we have two wave-functions over all space, $\psi(x)$ (in one dimension) and $\varphi(x)$. (The generalization to higher dimensions is straightforward.) It is frequently useful to determine the **dot product** of two wave-functions, which is a single complex number, defined as:

$$\psi \cdot \varphi = \int_{-\infty}^{\infty} \psi^*(x)\varphi(x)\, dx \qquad \text{(a complex number).}$$

Notice that the first wave-function, ψ, is conjugated. Now the bra representation of ψ^* is just $\langle\psi|$ and the ket representation of φ is $|\varphi\rangle$. When written next to each other, bra–ket combinations are defined as the dot product integral, i.e.,

$$\langle\psi|\varphi\rangle \equiv \psi \cdot \varphi = \int_{-\infty}^{\infty} \psi^*(x)\varphi(x)\, dx.$$

(A bra–ket combination is a bra–c–ket, < >. Get it?)

When writing a bra–ket combination, use only one vertical bar between them: $\langle\psi|\varphi\rangle$, *not* $\langle\psi||\varphi\rangle$.

As a related example, using our new Dirac shorthand, we can write the "squared-magnitude" (sometime called "squared-length") of ψ as the dot product of ψ with itself:

$$magnitude^2 = \int_{-\infty}^{\infty} \psi^*(x)\psi(x)\, dx = \langle\psi|\psi\rangle.$$

2.3.1.1 Summary of Kets and Bras

> The ket shorthand for $\psi(x)$ is $|\psi\rangle$. The bra shorthand for $\psi^*(x)$ is $\langle\psi|$. Combining a bra with a ket, $\langle\psi|\varphi\rangle$, invokes the dot product operation.

Quite simply, a **ket** is a function of space; a **bra** is the complex conjugate of such a function. A bra–ket is the dot product of the bra and ket, yielding a complex number. Recall that the QM dot product is *not* commutative (discussed elsewhere):

$$\langle\psi|\varphi\rangle \equiv \int_{-\infty}^{\infty} \psi^*(x)\varphi(x)\, dx = \langle\varphi|\psi\rangle^*$$

(reversing the operands conjugates the dot product).

We have seen that kets and bras can be wave-functions which are quantum states, but as noted earlier, kets and bras are more general than that. A ket or a bra can be either a quantum state, or the result of *operations* on a state. In other words, a ket or bra can be most any function of space. (Recall that a **quantum state** defines everything there is to know about a particle, including probabilities of finding it anywhere in space. A particle spatial quantum state (i.e., excluding its spin part), can be expressed as a complex-valued function of position, say $\psi(x,y,z)$.) Therefore,

> All states are kets, but not all kets are states.

For example, a particle can be in a *state* $|\psi\rangle$, but no particle state can be given by the *ket* $\hat{p}|\psi\rangle$.

A note about spin: Wave-functions alone may not fully define a quantum state, because they do not define the **spin** of a particle, i.e., its intrinsic angular momentum. Therefore, a full quantum state, for a particle with spin, is a combination of the wave-function (spatial state) and its **spin-state**. More on this later.

2.3.2 Operators in Dirac Notation

This section repeats much of the information in the previous “Operators” section, but in Dirac notation.

An operator acting on a ket $|\psi\rangle$ *produces another ket.* The given ket $|\psi\rangle$ may or may not be a *state*, and the resulting ket may or may not be a *state*, i.e., it may or may not represent a quantum state that a system could be in. If a result ket is not a state, then what is it? It may be a linear combination (superposition) of results, computed from operators acting on a superposition of states. It may be represented as a sum (superposition) of basis vectors:

$$\text{Given} \quad |\psi\rangle = \sum_{n=1}^{\infty} c_n |\phi_n\rangle, \quad \text{then} \quad \hat{o}|\psi\rangle = \sum_{n=1}^{\infty} c_n \hat{o} |\phi_n\rangle.$$

In any case, it is a vector in the ket vector-space that contains information of interest.

An operator acts on a ket to produce another ket. Either one or both kets may or may not be "states."

A linear operator acting on a *state* $|\psi\rangle$ produces a superposition of *results* based on the superposition of *states* composing $|\psi\rangle$.

Some references do not properly distinguish between a "ket" and a "state." Some even go so far as to define an "operator" as acting on a "state" to produce another "state." This is wrong.

A linear operator acting on a nonstate ket produces a superposition of new results based on the superposition of prior results composing the given ket.

Recall that in Dirac notation, kets and bras are independent of the representation basis. For Dirac algebra to work, operators must also be independent of representation. Therefore, Dirac operators never have things like $\partial/\partial x$, because that implies a specific representation basis. Instead, Dirac operators are just labels that describe their function, but the actual implementation of an operator in any basis is not specified. That is the beauty of Dirac algebra: much of the tedium of complicated operators is eliminated. The algebra works by universal identities and properties of kets, bras, and operators.

Dirac operators may be written three ways: preceding a ket, between a bra and a ket, and less often, following a bra with nothing to the right:

$\hat{o}|\psi\rangle$	means the operator "$\hat{o}$" acting on the ket "$|\psi\rangle$."
$\langle\varphi|\hat{o}|\psi\rangle$	means the dot product of $\langle\varphi|$ with the result of "$\hat{o}$" acting on $|\psi\rangle$.
$\langle\psi|\hat{o}$	means the operator acting to the left, $\left(\hat{o}^\dagger|\psi\rangle\right)^\dagger$, which is a bra.

This last case of a lone operator following a bra is interpreted as the left-action of the operator on the bra. We usually think of operators as acting on the ket to the right, but there is also a way of defining the action of an operator on the bra to the left [16, p. 15m]. Adjoints and left-action are discussed on p. 66.

Here is an example of Dirac algebra using operator algebra and kets and bras. Consider the energy eigenstates (stationary states) of a harmonic oscillator, $|u_0\rangle, |u_1\rangle, |u_2\rangle, \ldots$, and the lowering operator, $\hat{a}$. What is the result of "$\hat{a}$" on a ket $|u_n\rangle$? In other words, what is $\hat{a}|u_n\rangle$? We can answer that question with Dirac algebra, by starting with an identity for the lowering operator:

$$\text{Given:} \quad \langle u_{n-1}|\hat{a}|u_n\rangle = \sqrt{n}, \quad \forall n, \qquad \text{and} \quad \langle u_j|\hat{a}|u_n\rangle = 0, \quad j \neq n-1.$$

This implies that $\hat{a}|u_n\rangle$ is a multiple of $|u_{n-1}\rangle$. Then from the first identity, we must have:

$$\langle u_{n-1}|\hat{a}|u_n\rangle = \sqrt{n}\langle u_{n-1}|u_{n-1}\rangle \qquad \text{since } \langle u_{n\text{-}1}|u_{n\text{-}1}\rangle = 1 \quad \text{(basis functions normalized).}$$

Now "divide" both sides by $\langle u_{n-1}|$:

$$\hat{a}|u_n\rangle = \sqrt{n}|u_{n-1}\rangle.$$

The "divide" is only possible because all other inner products are zero in the "givens." Note that non-Hermitian operators such as this are calculation aids and nothing more.

Composition of Operators: Two operators may be composed, i.e., the first acts on a ket to produce another ket, then the second acts on the result of the first. For example, $\hat{g}\hat{h}|\psi\rangle$ means $\hat{g}$ acts on the result of $\hat{h}$ acting on $|\psi\rangle$. The combination $\hat{g}\hat{h}$ "looks like" multiplying $\hat{g}$ and $\hat{h}$, but it is not. It is the **composition** of $\hat{g}$ on $\hat{h}$. Sometimes, references even call such a composition "$\hat{g}$ times $\hat{h}$," but there may not be any multiplication involved.

For scalar multiplication, such as $ab|\psi\rangle$, where "a" and "b" are complex numbers, then "a" and "b" are, in fact, multiplied. Also, for finite state spaces, where $\hat{g}$ and $\hat{h}$ are matrices, the composition is, indeed, matrix multiplication.

Summary: An operation on a quantum state is not necessarily a quantum state, but the result *is* a function of space. Therefore, it can be represented by a ket (or bra). In other words, the result of an operator on a ket is another ket, e.g., $\hat{o}|\psi\rangle$ is the operator "$\hat{o}$" on the ket $|\psi\rangle$ and is itself a ket. This resulting ket is often not a quantum state (i.e., it does not completely define all the properties of any particle), but it is still a useful function of all space. A linear operator acting on a state $|\psi\rangle$ produces a superposition of results based on the superposition of states which compose $|\psi\rangle$.

In the case of operators for observables, as we have seen, an operator "brings out" some physical property from a quantum state, such as the energy of the particle, or its position, or its momentum. But the computation can only be completed by taking a relevant inner product of a bra with the result of the operator acting on the state.

In some cases, however, an operator converts a state into another state, such as the time evolution operator, a translation operator, or a rotation operator. In other cases, Springer

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